

CLAIMS

What is claimed is:

1. A blocked mercaptosilane selected from the group consisting of:

2. $[(ROC(=O))_p(G)_j]_k - Y - S - G - (SiX_3)_n$ (1); and

3. $[(X_3Si)_q - G]_s - [Y - [S - G - SiX_3]_b]_c$ (2)

4. wherein

5. Y is a polyvalent species $(Q)_zA(=E)$ selected from the group consisting of $-C(=NR)-$;
 6. $-SC(=NR)-$; $-SC(=O)-$; $-OC(=O)-$; $-S(=O)-$; $-S(=O)_2-$; $-OS(=O)_2-$; $(-NR)S(=O)_2-$; $-SS(=O)-$;
 7. $-OS(=O)-$; $(-NR)S(=O)-$; $-SS(=O)_2-$; $(-S)_2P(=O)-$; $(-S)P(=O)(-)-$; $(-S)_2P(=S)-$;
 8. $(-S)P(S)-$; $P(S)(-)-$; $(-NR)_2P(=O)-$; $(-NR)(-S)P(=O)-$; $(-O)(-NR)P(=O)-$; $(-O)(-S)P(=O)-$;
 9. $(-O)_2P(=O)-$; $(-O)P(=O)-$; $(-NR)P(=O)-$; $(-NR)_2P(=S)-$; $(-NR)(-S)P(=S)-$; $(-O)(-NR)P(=S)-$;
 10. $(-O)(-S)P(=S)-$; $(-O)_2P(=S)-$; $(-O)P(=S)-$; and $(-NR)P(=S)-$; wherein the atom A attached to
 11. unsaturated heteroatom E is attached to the sulfur which in turn is linked via a group G to the
 12. silicon atom;

13. each R is chosen independently from hydrogen, straight, cyclic, or branched alkyl that
 14. may or may not contain unsaturation, alkenyl groups, aryl groups, and aralkyl groups, with
 15. each R containing from 1 to 18 carbon atoms;

16. each G is independently a monovalent or polyvalent group derived by substitution of
 17. alkyl, alkenyl, aryl, or aralkyl, wherein G can contain from 1 to 18 carbon atoms, and if G is
 18. univalent, G can be a hydrogen atom;

19. X is independently selected from the group consisting of $-Cl$, $-Br$, $RO-$, $RC(=O)O-$,
 20. $R_2C=NO-$, R_2NO- , R_2N- , $-R$, and $-(OSiR_2)_2(OSiR_3)$ wherein each R is as above and at least
 21. one X is not $-R$;

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22 p is 0 to 5; r is 1 to 3; z is 0 to 2; q is 0 to 6; a is 0 to 7; b is 1 to 3; j is 0 to 1, but it
23 may be 0 only if p is 1; c is 1 to 6; t is 0 to 5; s is 1 to 3; k is 1 to 2; with the provisos that (I) if
24 A is carbon, sulfur or sulfonyl, then (i) a + b is 2 and (ii) k is 1; (II) if A is phosphorus, then
25 a + b is 3 unless both (i) c is greater than 1 and (ii) b is 1, in which case a is c + 1; and (III) if
26 A is phosphorus, then k is 2.

1 2. A blocked mercaptosilane according to claim 1 wherein R is selected from the group
2 consisting of methyl, ethyl, propyl, isobutyl, phenyl, tolyl, phenethyl, norbornyl, norbornenyl,
3 ethylnorbornyl, ethylnorbornenyl, ethylcyclohexyl, ethylcyclohexenyl, and
4 cyclohexylcyclohexyl.

1 3. A blocked mercaptosilane according to claim 1 according to formula (I).

1 4. A blocked mercaptosilane according to claim 1 according for formula (II).

1 5. A blocked mercaptosilane according to claim 1 which has been partially hydrolyzed.

1 6. A blocked mercaptosilane according to claim 1 wherein Y is selected from the group
2 consisting of: -OC(=O)-; -SC(=O)-; -S(=O)-; -OS(=O)-; -(S)P(=O)-; and -P(=O)(-)2.

1 7. The blocked mercaptosilane of claim 1 wherein Y is selected from the group consisting
2 of -C(=NR)- and -SC(=NR)-.

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1 8. The blocked mercaptosilane of claim 1 wherein Y is selected from the group consisting
2 of -S(=O)₂-; -OS(=O)₂-; (-NR)S(=O)₂-; -SS(=O)-; (-NR)S(=O)-; and -SS(=O)₂-.

1 9. The blocked mercaptosilane of claim 1 wherein Y is selected from the group consisting
2 of (-S)₂P(=O)-; (-S)₂P(=S)-; -(S)P(=S)-; -P(=S)(-); (-NR)₂P(=O)-; (-NR)(-S)P(=O)-;
3 (-O)(-NR)P(=O)-; (-O)(-S)P(=O)-; (-O)₂P(=O)-; -(O)P(=O)-; -(-NR)P(=O)-; (-NR)₂P(=S)-;
4 (-NR)(-S)P(=S)-; (-O)(-NR)P(=S)-; (-O)(-S)P(=S)-; (-O)₂P(=S)-; -(O)P(=S)-; and
5 -(-NR)P(=S)-.

1 10. A blocked mercaptosilane according to claim 1 wherein the sum of the carbon atoms
2 within the G groups within the molecule is from 3 to 18.

1 11. A blocked mercaptosilane according to claim 1 wherein X is selected from the group
2 consisting of methoxy, ethoxy, isobutoxy, propoxy, isopropoxy, acetoxy, and oximato.

1 12. A blocked mercaptosilane according to claim 1 wherein p is 0 to 2; X is RO- or
2 RC(=O)O-; R is selected from the group consisting of hydrogen, phenyl, isopropyl,
3 cyclohexyl, isobutyl; and G is a substituted phenyl or substituted straight chain alkyl of C₂ to
4 C₁₂.

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1 13. A blocked mercaptosilane of the formula: $X_3SiGSC(=O)GC(=O)SGSiX_3$ wherein
2 each R is chosen independently from hydrogen, straight, cyclic, or branched alkyl that
3 may or may not contain unsaturation, alkenyl groups, aryl groups, and aralkyl groups, with
4 each R containing from 1 to 18 carbon atoms;
5 each G is independently a divalent group derived by substitution of alkyl, alkenyl, aryl,
6 or aralkyl, wherein G can contain from 1 to 18 carbon atoms, with the proviso that G is not
7 such that the blocked mercaptosilane would contain an α,β -unsaturated carbonyl including a
8 carbon-carbon double bond next to the thiocarbonyl group;

X is independently selected from the group consisting of -Cl, -Br, RO-, RC(=O)O-,

¹⁰* R₂C=NO-, R₂NO-, R₂N-, -R, and -(OSiR₂)_i(OSiR₃) wherein each R is as above and at least one X is not -R; and

X is not -R; and

t is 0 to 5

14. A blocked mercaptosilane selected from the group consisting of:

2	$[(ROC(=O))_p(G)_j]_k-Y-S]_r-G-(SiX_3)_s$	(1); and
3	$[X_3Si]_q-G]_a-[Y-S-G-SiX_3]_b]_c$	(2)
4	wherein	

Y is a -C(=O)-;

each R is chosen independently from hydrogen, straight, cyclic, or branched alkyl that
may or may not contain unsaturation, alkenyl groups, aryl groups, and aralkyl groups, with
each R containing from 1 to 18 carbon atoms;

each G is independently a monovalent or polyvalent group derived by substitution of
alkyl, alkenyl, aryl, or aralkyl, wherein G can contain from 1 to 18 carbon atoms, with the

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11 proviso that G is not such that the blocked mercaptosilane would contain an α,β -unsaturated
12 carbonyl including a carbon-carbon double bond that can undergo polymerization reactions
13 next to the thiocarbonyl group;

14 X is independently selected from the group consisting of -Cl, -Br, RO-, RC(=O)O-,
15 R₂C=NO-, R₂NO-, R₂N-, -R, and -(OSiR₂)₂(OSiR₃), wherein each R is as above and at least
16 one X is not -R; and

17 p is 0 to 5; r is 1 to 3; q is 0 to 6; a is 0 to 1; b is 1 to 2; j is 1; c is 1 to 6; t is 0 to 5; s
18 is 1 to 3; k is 1; and a + b is 2.

15. The blocked mercaptosilane of claim 14 wherein p is 2 to 5.

16. The blocked mercaptosilane of claim 14 wherein G, which is directly bonded to Y, is
alkyl of from two to twelve carbon atoms.

1 17. The blocked mercaptosilane of claim 14 wherein G, which is directly bonded to Y, is
2 alkyl of from six to eight carbon atoms.

1 18. The blocked mercaptosilane of claim 14 wherein R is hydrogen or an alkyl having from
2 one to four carbon atoms.

1 19. The blocked mercaptosilane of claim 14 which has been partially hydrolyzed.

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8 atom;

9 each R is chosen independently from hydrogen, straight, cyclic or branched alkyl that

10 may or may not contain unsaturation, alkenyl groups, aryl groups, and aralkyl groups, with

11 each R containing from 1 to 18 carbon atoms;

12 each G is independently a monovalent or polyvalent group derived by substitution of

13 alkyl, alkenyl, aryl or aralkyl wherein G can contain from 1 to 18 carbon atoms, with the

14 proviso that if Y is -C(=O)-, G is not such that the blocked mercaptosilane would contain an
15 α,β -unsaturated carbonyl, and if G is univalent, G can be a hydrogen atom;

16 X is independently a group selected from the group consisting of -Cl, -Br, RO-,
17 RC(=O)O-, R₂C=NO-, R₂NO-, R₂N-, -R, and -(OSiR₂)_j(OSiR₃) wherein each R is as above
18 and at least one X is not -R;

19 Q is oxygen, sulfur or (-NR-);

20 A is carbon, sulfur, phosphorus, or sulfonyl;

21 E is oxygen, sulfur or NR;

22 p is 0 to 5; r is 1 to 3; z is 0 to 2; q is 0 to 6; a is 0 to 7; b is 1 to 3; j is 0 to 1, but it

23 may be 0 only if p is 1, c is 1 to 6, t is 0 to 5; s is 1 to 3; k is 1 to 2, with the provisos that (A)

24 if A is carbon, sulfur or sulfonyl, then (i) a + b = 2 and (ii) k = 1; (B) if A is phosphorus, then a

25 + b = 3 unless both (i) c is greater than 1 and (ii) b is 1, in which case a is c + 1; and (C) if A is

26 phosphorus, then k is 2.

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1 26. The composition of claim 25 wherein the carrier is a filler.

2 27. The composition of claim 26 wherein the filler is selected from the group consisting of
3 silica and carbon black.

10 28. The composition of Claim 25 wherein Y is selected from the group consisting of
-C(=NR)-; -SC(=NR)-; -C(=O)-; -SC(=O)-; -OC(=O)-; -S(=O)-; -S(=O)₂-; -OS(=O)₂-; (-
NR)S(=O)₂-; -SS(=O)-; -OS(=O)-; (-NR)S(=O)-; -SS(=O)₂-; (-S)₂P(=O)-; -(-S)P(=O)-;
-P(=O)(-); (-S)₂P(=S)-; -(-S)P(=S)-; -P(=S)(-); (-NR)₂P(=O)-; (-NR)(-S)P(=O)-;
(-O)(-NR)P(=O)-; (-O)(-S)P(=O)-; (-O)P(=O)-; -(-O)P(=O)-; -(-NR)P(=O)-; (-NR)P(=S)-;
(-NR)(-S)P(=S)-; (-O)(-NR)P(=S)-; (-O)(-S)P(=S)-; (-O)₂P(=S)-; -(-O)P(=S)-; and
-(-NR)P(=S)-.

1 29. The composition of Claim 25 wherein Y is -C(=O)-.

1 30. The composition of claim 26 which is the reaction product of the filler and the blocked
2 mercaptosilane.

1 31. The composition of claim 30 wherein the filler and blocked mercaptosilane are reacted
2 through the SiX₃ group of the blocked mercaptosilane.

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1 32. The composition of claim 25 wherein the carrier is a porous polymer.